

Recursive calculation of matrix elements for the generalized seniority shell model

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Abstract

A recursive calculational scheme is developed for matrix elements in the generalized seniority scheme for the nuclear shell model. Recurrence relations are derived which permit straightforward and efficient computation of matrix elements of one-body and two-body operators and basis state overlaps.

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1. Introduction

The generalized seniority [1, 2] or broken pair [3, 4] approximation provides a truncation scheme for the nuclear shell model, based on the dominance of like-nucleon pairing effects in semimagic (or nearly semimagic) nuclei. The fundamental premise is that there exists an energetically favored collective S pair, which can be constructed from like nucleons coupled to angular momentum zero, and that the ground state of an even-even nucleus can be well approximated by a condensate of such collective pairs. Low-lying excited states may then be obtained by breaking one or more S pairs. The resulting states are classified by the generalized seniority v , defined as the number of valence nucleons not participating in a collective S pair. The generalized seniority approach effectively reduces the dimensionality of the n -particle valence shell model to that of a v -particle shell model problem. In practice, such generalized seniority shell model calculations have been carried out for $v \leq 4$ (*e.g.*, Refs. [5–9]).

Moreover, the generalized seniority scheme provides a microscopic foundation for the phenomenologically successful interacting boson model (IBM) [10] and, for odd-mass and odd-odd nuclei, the interacting boson fermion model (IBFM) [11]. In this context, generalized seniority states constructed from the S pair and a collective D pair (consisting of like nucleons coupled to angular momentum 2) are mapped onto IBM states built from analogous combinations of s and d bosons [12–16]. The need for a fully microscopic derivation of the IBM Hamiltonian parameters and transition operators is a longstanding problem. A well-developed microscopic mapping would be especially valuable for the IBFM, where the relevance of single-particle degrees of freedom is particularly manifest.

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For instance, higher-order mapping from the generalized seniority shell model space onto the IBFM would facilitate the prediction of collective effects in β decay [17]. The need is also emphasized by recent applications of the model to neutrinoless double beta decay [18], where phenomenological calibration of the model is not a viable alternative. For microscopic derivation of the IBM and IBFM, matrix elements of various operators between states of generalized seniority $v \lesssim 6$ are of interest.

In addition to matrix elements of operators between generalized seniority states, it is also necessary to compute the overlaps of these states, since the canonical construction [3] leads to a nonorthogonal basis. The S pair creation operator is obtained as a linear combination of pair creation operators for each active single-particle level (*i.e.*, j shell). The individual j shells may be treated using the conventional seniority or quasispin results [19, 20]. Then, the overlaps and matrix elements in the generalized seniority scheme may in principle be computed from the single-shell results by combinatorial arguments [3, 13, 21].

However, the combinatorial derivation [13] rapidly becomes cumbersome with increasing generalized seniority. It was noted [22] that commutator methods can be used to obtain simplifications, but the resulting hybrid approach could still only be practically applied for $v \leq 2$ [22, 23]. The main challenge in proceeding to higher generalized seniority lies in accounting for the intermediate angular momentum couplings which occur among the particles not participating in the collective S pair. Several approaches have been pursued. The combinatorial approach may be pushed further by introducing certain simpler intermediate quantities, essentially norms for uncoupled states, and then reexpressing the overlaps for the angular-momentum coupled states in terms of these (however, matrix elements were not explicitly considered in this formulation) [24]. One may directly carry out the calculations of overlaps and matrix elements by Wick's theorem in an uncoupled scheme, subsequently recoupling the results [25]. An alternative, indirect construction of the generalized seniority basis relies upon number projection of generalized-quasiparticle states involving complex parameters. Matrix elements are then evaluated as contour integrals in the complex plane [4, 5, 26]. These latter methods have been applied for $v \lesssim 4$.

In the present work, a systematic calculational scheme is established, in which recurrence relations for the matrix elements and overlaps are derived by angular-momentum coupled commutator methods [27, 28]. This is essentially a Wick's theorem approach, which, however, retains the angular-momentum coupled structure. General expressions are obtained by which the one-body operator matrix elements and the overlaps for states of generalized seniority v and pair number N are expressed in terms of commutators which yield matrix elements and overlaps involving lower values of v and/or N . The explicit recurrence relations to be used in the numerical calculations for a *specific* value of the generalized seniority are obtained from these generic expressions by a straightforward procedure involving repeated application of a commutator product rule. The matrix elements of two-body operators can be computed directly in terms of these basic one-body operator matrix elements and overlaps. An essential motivation for the present approach is that calculation can proceed to higher generalized seniority in a methodical fashion, through systematic application of this coupled commutator product rule, and that the process is readily amenable to automation [29]. For illustration, the explicit recurrence relations are given for matrix elements and overlaps involving low generalized seniority states, sufficient for generalized seniority shell model calculations with $v \leq 3$. In

particular, calculation of the matrix elements of a two-body Hamiltonian between states of $v = 3$ requires one-body operator matrix elements for $v \leq 4$ and overlaps for $v \leq 5$.

After a review of definitions (Sec. 2), the general commutation scheme is outlined (Sec. 3), and the underlying commutator algebra results are summarized (Sec. 4). A coupled set of recurrence relations for the one-body operator matrix elements (Sec. 5) and overlaps (Sec. 6) are obtained. Matrix elements of two-body operators are then expressed in terms of these quantities (Sec. 7).

2. Definitions

First, let us review the definitions necessary for the generalized seniority scheme. Within a single major shell, the angular-momentum label is sufficient to uniquely specify a single-particle level, so let $C_{c,\gamma}^\dagger$ be the creation operator for a particle in the state of angular momentum c and z -projection quantum number γ .¹ The angular-momentum coupled product of two spherical tensor operators is defined by $(A^a \times B^b)_\gamma^c = \sum_{\alpha\beta} (a\alpha b\beta | c\gamma) A_\alpha^a B_\beta^b$, and we follow the time reversal phase convention $\tilde{A}_\alpha^a = (-)^{a-\alpha} A_{-\alpha}^a$ [30]. Then the angular-momentum coupled pair creation operator is defined by

$$A_{ab}^{e\dagger} = (C_a^\dagger \times C_b^\dagger)^e, \quad (1)$$

and its time-reversed adjoint is $\tilde{A}_{ab}^e \equiv \widetilde{(A_{ab}^{e\dagger})^\dagger} = -(\tilde{C}_a \times \tilde{C}_b)^e$.

The state of zero generalized seniority is defined by the S -pair condensate, $|S^N\rangle = S^{\dagger N}|0\rangle$, where the collective S pair in the generalized seniority scheme is defined by

$$S^\dagger = \sum_c \alpha_c \frac{\hat{c}}{2} A_{cc}^{0\dagger}, \quad (2)$$

with $\hat{c} = (2c+1)^{1/2}$. The amplitudes α_c are conventionally taken subject to the normalization condition $\sum_c (2c+1)\alpha_c^2 = \sum_c (2c+1)$. They may be obtained by a variety of prescriptions [1, 3, 25, 31, 32], for instance, variationally so as to minimize the energy expectation value $\langle S^N | H | S^N \rangle$.

More generally, a state of generalized seniority v is constructed as $|S^N F^f\rangle = S^{\dagger N} F^{f\dagger} |0\rangle$, where the fermion cluster $F^{f\dagger}$ is a product of v creation operators, coupled to total angular momentum f . A complete set of such clusters is constructed by successive couplings of the form $F^f = ((A^\dagger \times A^\dagger) \cdots \times A^\dagger)^f$ for v even or $F^f = (((A^\dagger \times A^\dagger) \cdots \times A^\dagger) \times C^\dagger)^f$ for v odd. In particular, the conventional microscopic interpretation [14] of the IBM is formulated in terms of generalized seniority states involving the collective D pair, defined as a general linear combination

$$D^\dagger = \sum_{\substack{ab \\ a \leq b}} \frac{\beta_{ab}}{(1 + \delta_{ab})^{1/2}} A_{ab}^{2\dagger}, \quad (3)$$

¹For simplicity of notation, we do not distinguish between the level c and its angular momentum j_c . Also note that, following Ref. [28], we denote operators by capital roman letters, angular momenta by lower case roman letters, and angular-momentum z -projection quantum numbers, when needed, by the corresponding lower case Greek letter (*e.g.* A_α^a , B_β^b , C_γ^c).

of pairs of angular momentum 2. The states of interest for mapping from the shell model to the IBM, through the Otsuka-Arima-Iachello (OAI) mapping [12–16], are of the form $|S^N\rangle, |S^N D\rangle, |S^N(DD)^f\rangle$, *etc.* For the analogous mapping [33] to the IBFM, the relevant states are $|S^N C_a\rangle, |S^N(DC_a)^f\rangle$, *etc.* Any matrix element or overlap involving D pairs may be expanded in terms of those for the elementary pairs A_{ab}^2 , through (3).

The matrix elements of most immediate interest are those of one-body and two-body operators. Any spherical tensor one-body operator may be expressed in terms of the elementary one-body multipole operators

$$T_{rs}^t = (C_r^\dagger \times \tilde{C}_s)^t, \quad (4)$$

through the usual second-quantized realization, which in angular-momentum coupled form becomes $U^u = -\sum_{ab} \hat{u}^{-1} \langle a \| U^u \| b \rangle T_{ab}^u$.² Thus, we must consider matrix elements of T_{rs}^t taken between states of the generalized seniority scheme, which are of the form $\langle S^N G^g \| T_{rs}^t \| S^N F^f \rangle$, where F^f and G^g represent clusters of v nucleons not participating in the collective S pairs. Since the generalized seniority states are not orthonormal, as canonically constructed in terms of clusters above [15], it is also necessary to compute the norms and overlaps $\langle S^N G^f | S^N F^f \rangle$.

The creation operators for the generalized seniority basis states, as defined above, have a uniform structure consisting of sequentially coupled pair creation operators (with a single additional creation operator in the case of odd v). Therefore, it is more compact and readable to simply label these states by the single-particle level labels and the angular momenta for intermediate couplings, that is, as $|S^N\rangle \equiv S^{\dagger N} |0\rangle$, $|S^N c\rangle \equiv S^{\dagger N} C_c^\dagger |0\rangle$, $|S^N(ab)^e\rangle \equiv S^{\dagger N} A_{ab}^{e\dagger} |0\rangle$, $|S^N(ab)^e i^g\rangle \equiv S^{\dagger N} (A_{ab}^{e\dagger} \times C_i^g) |0\rangle$, $|S^N(ab)^e (ij)^{mg}\rangle \equiv S^{\dagger N} (A_{ab}^{e\dagger} \times A_{ij}^{m\dagger})^g |0\rangle$, *etc.*

Only matrix elements and overlaps involving bra and ket states of *equal* generalized seniority need be calculated explicitly through recurrence relations. To facilitate writing (and discussing) the recurrence relations, we furthermore introduce the symbol $O_N^{(v)}[\dots]$ for the overlaps of states of equal generalized seniority v , as

$$\begin{aligned} O_N^{(0)} &\equiv \langle S^N | S^N \rangle \\ O_N^{(1)}[c|c] &\equiv \langle S^N c | S^N c \rangle \\ O_N^{(2)}[(cd)^e|(ab)^e] &\equiv \langle S^N(cd)^e | S^N(ab)^e \rangle \\ O_N^{(3)}[(cd)^f j^g|(ab)^e i^g] &\equiv \langle S^N(cd)^f j^g | S^N(ab)^e i^g \rangle \\ O_N^{(4)}[(cd)^f (kl)^{ng} |(ab)^e (ij)^{mg}] &\equiv \langle S^N(cd)^f (kl)^{ng} | S^N(ab)^e (ij)^{mg} \rangle, \end{aligned} \quad (5)$$

etc. Similarly, we introduce $T_N^{(v)}[\dots]$ for the one-body operator matrix elements between these states, *e.g.*,

$$T_N^{(4)}[(cd)^f (kl)^{nh} |(rs)^t |(ab)^e (ij)^{mg}] \equiv \langle S^N(cd)^f (kl)^{nh} \| T_{rs}^t \| S^N(ab)^e (ij)^{mg} \rangle. \quad (6)$$

These definitions are intended to follow the bracket notation as closely as possible, while clearly exhibiting the labels v and N with respect to which the recurrence will be carried

²However, in comparing with, *e.g.*, Ref. [34], note that the overall sign of this expression varies depending upon the time-reversal phase convention, presently $\hat{A}_\alpha^a = (-)^{a-\alpha} A_{-\alpha}^a$.

out, and also more simply laying out the arguments of $O_N^{(v)}$ and $T_N^{(v)}$ considered as symbols in the recursive computational scheme.

Matrix elements or overlaps involving states of *unequal* generalized seniority can readily be expressed in terms of these by expanding one or more S pairs in terms of the pairs $(aa)^0$, *i.e.*, created by $A_{aa}^{0\dagger}$, for individual j shells, according to the definition (2), *e.g.*,

$$\langle S^N(cd)^g | S^{N-1}(ab)^e (ij)^{mg} \rangle = \sum_k \alpha_k \frac{\hat{k}}{2} O_{N-1}^{(4)}[(kk)^0 (cd)^g | (ab)^e (ij)^{mg}]. \quad (7)$$

Here we notice that, although the pair $(kk)^0$ carries *seniority* zero, it is not the *collective* S pair and therefore carries a *generalized* seniority of 2.

It should be noted that the $T_N^{(v)}$ and $O_N^{(v)}$ obey a variety of symmetry relations under rearrangement of the arguments, and therefore they need not all be calculated independently. For instance, different orderings of single-particle labels within the bra or ket are related by, *e.g.*, $A_{ba}^{e\dagger} = -\theta(abe)A_{ab}^{e\dagger}$ and $(A_{ab}^{e\dagger} \times A_{ij}^{m\dagger})^g = \theta(emg)(A_{ij}^{m\dagger} \times A_{ab}^{e\dagger})^g$, where

$$\theta(abc \dots) = (-)^{a+b+c+\dots}. \quad (8)$$

Thus, for instance,

$$T_N^{(4)}[(cd)^f (kl)^{nh} | (rs)^t | (ab)^e (ij)^{mg}] = -\theta(abe) T_N^{(4)}[(cd)^f (kl)^{nh} | (rs)^t | \overleftrightarrow{(ba)^e (ij)^{mg}}], \quad (9)$$

interchanging particles within a pair, as indicated by the arrows, or

$$T_N^{(4)}[(cd)^f (kl)^{nh} | (rs)^t | (ab)^e (ij)^{mg}] = \theta(emg) T_N^{(4)}[(cd)^f (kl)^{nh} | (rs)^t | \overleftrightarrow{(ij)^m (ab)^e g}], \quad (10)$$

interchanging pairs within a cluster. Moreover, the property of the reduced matrix element under complex conjugation, $\langle c || B^b || a \rangle^* = (-)^{a+b-c} \langle a || \tilde{B}^{b\dagger} || c \rangle$, gives the relation

$$\langle S^N G^g || T_{rs}^t || S^N F^f \rangle = -(-)^{r+s+g-f} \langle S^N F^f || T_{sr}^t || S^N G^g \rangle, \quad (11)$$

where we note that $\tilde{C}_c^\dagger = -C_c^\dagger$, and consequently $\tilde{T}_{rs}^{t\dagger} = -\theta(rst)T_{sr}^t$. Thus, for instance,

$$T_N^{(4)}[(cd)^f (kl)^{nh} | (rs)^t | (ab)^e (ij)^{mg}] = -\theta(rsg) T_N^{(4)}[(ab)^e (ij)^{mg} | \overleftrightarrow{(sr)^t (cd)^f (kl)^{nh}}], \quad (12)$$

interchanging bra and ket and conjugating the operator.

3. General scheme for recurrence

Recurrence relations for the reduced matrix elements and overlaps can be naturally derived by commutator methods. These matrix elements and overlaps must first be expressed as vacuum expectation values of coupled products of creation and annihilation operators. The operators are then reordered, by making use of their commutation (or anticommutation) relations, until all the resulting terms themselves represent matrix elements or overlaps of generalized seniority states. Since the commutators (or anticommutators) yield terms with *fewer* total creation and annihilation operators, the matrix

elements and overlaps resulting from these terms will automatically involve states of lower pair number or generalized seniority, thus giving rise to relations which are recursive with respect to N or v .

In general, consider two states $|A_\alpha^a\rangle = A_\alpha^{a\dagger}|0\rangle$ and $|C_\gamma^c\rangle = C_\gamma^{c\dagger}|0\rangle$, obtained by the action of some operators $A_\alpha^{a\dagger}$ and $C_\gamma^{c\dagger}$ on the vacuum, for instance, coupled products of fermion creation operators. Then the reduced matrix element of an operator B^b can be reexpressed as the vacuum expectation value

$$\langle C^c \| B^b \| A^a \rangle = (-)^{a-b-c} \langle 0 | [\tilde{C}^c \times (B^b \times A^{a\dagger})^c]_0^0 | 0 \rangle \quad (13)$$

of a scalar triple product of operators.³ The overlap $\langle B^a | A^a \rangle \equiv \langle B_\alpha^a | A_\alpha^a \rangle$ of two states can similarly be evaluated as the vacuum expectation value

$$\langle B^a | A^a \rangle = \hat{a}^{-1} \langle 0 | (\tilde{B}^a \times A^{a\dagger})_0^0 | 0 \rangle. \quad (14)$$

The matrix element of the one-body operator T_{rs}^t between states of generalized seniority v is therefore given by an expression of the form

$$\langle S^N G^g \| T_{rs}^t \| S^N F^f \rangle = (-)^{f-t-g} \langle 0 | (\tilde{G}^g \tilde{S}^N \times T_{rs}^t \times S^{\dagger N} F^{f\dagger})^0 | 0 \rangle, \quad (15)$$

where $F^{f\dagger}$ and $G^{g\dagger}$ represent two clusters consisting of v fermionic creation operators. The overlap of two states of generalized seniority v is similarly

$$\langle S^N G^f | S^N F^f \rangle = \hat{f}^{-1} \langle 0 | (\tilde{G}^f \tilde{S}^N \times S^{\dagger N} F^{f\dagger})^0 | 0 \rangle, \quad (16)$$

where again $F^{f\dagger}$ and $G^{f\dagger}$ represent two clusters consisting of v fermionic creation operators, now with the same angular momentum $f = g$.

To outline the general scheme for deriving the recurrence relation for a matrix element $T_N^{(v)}$, let us momentarily suppress the details of angular-momentum coupling, the single-particle level labels, and the various numerical coefficients. To highlight the rearrangement taking place in each step, the factors to be reordered are indicated by an underbrace, and the general form of the commutator introduced by this reordering (if the factors do not freely commute) is shown schematically underneath. It suffices to note that commutation of an operator T or \tilde{A} through $S^{\dagger N}$ will yield terms of the form $[T, S^{\dagger N}] \sim A^\dagger S^{\dagger N-1}$ [see (42) in Sec. 5] or $[\tilde{A}, S^{\dagger N}] \sim S^{\dagger N-1} + T S^{\dagger N-1} + S^{\dagger N-1} T$ [see (43) in Sec. 5]. The time reversed adjoint expressions (see Sec. 4) apply for commutation through \tilde{S}^N . Furthermore, new clusters will arise from commutation through the clusters F and G , specifically, with creation operators defined by $E^\dagger \sim [T, G^\dagger]$, $H^\dagger \sim [T, F^\dagger]$, and $I^\dagger \sim [\tilde{A}, G^\dagger]$, to be calculated as described in Sec. 4.

Beginning with the reduced matrix element $T_N^{(v)} = \langle S^N G \| T \| S^N F \rangle$, expressed as a vacuum expectation value as in (15), we set out to commute the one-body operator to

³Relation (13) is readily derived from the identity $\langle c \| B^b \| a \rangle = \sum_{\alpha\beta\gamma} (-)^{c-\gamma} \begin{pmatrix} c & b & a \\ -\gamma & \beta & \alpha \end{pmatrix} \langle c\gamma | B_\beta^b | a\alpha \rangle$ [35] and is the operator analog of, *e.g.*, (14.16) of Ref. [19]. We follow the normalization and phase convention of Refs. [30, 35] for the Wigner-Eckart theorem, *i.e.*, $\langle c\gamma | B_\beta^b | a\alpha \rangle = (-)^{2b} \hat{c}^{-1} (a\alpha b\beta | c\gamma) \langle c \| B^b \| a \rangle$.

the right, where it will annihilate the vacuum. Thus, factors must be reordered as

$$\begin{aligned}
T_N^{(v)} &\sim \langle 0 | (\tilde{G}\tilde{S}^N) \underbrace{T(S^{\dagger N} F^\dagger)}_{A^\dagger S^{\dagger N-1}} | 0 \rangle \\
&\sim \langle 0 | (\tilde{G}\tilde{S}^N) (S^{\dagger N} \underbrace{TF^\dagger}_{\equiv H^\dagger}) | 0 \rangle + \langle 0 | \tilde{G}\tilde{S}^N A^\dagger S^{\dagger N-1} F^\dagger | 0 \rangle \\
&\sim \langle 0 | (\tilde{G}\tilde{S}^N) (S^{\dagger N} H^\dagger) | 0 \rangle + \langle 0 | \tilde{G}\tilde{S}^N A^\dagger S^{\dagger N-1} F^\dagger | 0 \rangle.
\end{aligned} \tag{17}$$

The first term is recognized as the overlap $\langle S^N G | S^N H \rangle \sim \langle 0 | (\tilde{G}\tilde{S}^N) (S^{\dagger N} H^\dagger) | 0 \rangle$. Note that the cluster H again contains v fermions. To evaluate the second term, we must commute A^\dagger to the left, where it will eventually annihilate the vacuum, yielding

$$\begin{aligned}
&\langle 0 | \tilde{G} \underbrace{\tilde{S}^N A^\dagger}_{\tilde{S}^{N-1} + T\tilde{S}^{N-1} + \tilde{S}^{N-1}T} S^{\dagger N-1} F^\dagger | 0 \rangle \\
&\sim \langle 0 | (\underbrace{\tilde{G}A^\dagger}_{\equiv \tilde{I}} \tilde{S}^N) (S^{\dagger N-1} F^\dagger) | 0 \rangle + \langle 0 | (\tilde{G}\tilde{S}^{N-1}) (S^{\dagger N-1} F^\dagger) | 0 \rangle \\
&\quad + \langle 0 | (\underbrace{\tilde{G}T}_{\equiv \tilde{E}} \tilde{S}^{N-1}) (S^{\dagger N-1} F^\dagger) | 0 \rangle + \langle 0 | (\tilde{G}\tilde{S}^{N-1}) T (S^{\dagger N-1} F^\dagger) | 0 \rangle \\
&\sim \langle 0 | (\tilde{I}\tilde{S}^N) (S^{\dagger N-1} F^\dagger) | 0 \rangle + \langle 0 | (\tilde{G}\tilde{S}^{N-1}) (S^{\dagger N-1} F^\dagger) | 0 \rangle \\
&\quad + \langle 0 | (\tilde{E}\tilde{S}^{N-1}) (S^{\dagger N-1} F^\dagger) | 0 \rangle + \langle 0 | (\tilde{G}\tilde{S}^{N-1}) T (S^{\dagger N-1} F^\dagger) | 0 \rangle.
\end{aligned} \tag{18}$$

The first term is recognized as the overlap $\langle S^{N-1}(SI) | S^{N-1}F \rangle$, the second term as $\langle S^{N-1}G | S^{N-1}F \rangle$, the third term as $\langle S^{N-1}E | S^{N-1}F \rangle$, and the final term as $\langle S^{N-1}G | T | S^{N-1}F \rangle$. Note that each of the clusters E , H , and SI [where the S pair is expanded as in (7)] again contains v fermions. Therefore, the resulting recurrence relation has the form

$$T_N^{(v)} \sim O_N^{(v)} + T_{N-1}^{(v)} + O_{N-1}^{(v)}. \tag{19}$$

Similarly, a reduction in seniority v is then provided through the recurrence relation for the overlap $O_N^{(v)} = \langle S^N G | S^N F \rangle$. The overlap is expressed as a vacuum expectation value as in (16), and a fermion is “decoupled” from each of the initial clusters F and G , leaving behind a subcluster of reduced seniority, denoted by H or I , *i.e.*, $F^\dagger \sim C^\dagger H^\dagger$ and $G^\dagger \sim C^\dagger I^\dagger$. These fermion operators are then migrated inwards and recoupled to constitute a one-body operator, thereby yielding the reduced matrix element of a one-body operator, but now of lower seniority. Schematically,

$$\begin{aligned}
O_N^{(v)} &\sim \langle 0 | (\tilde{G}\tilde{S}^N) (S^{\dagger N} F^\dagger) | 0 \rangle \\
&\sim \langle 0 | (\tilde{I} \underbrace{\tilde{C}\tilde{S}^N}_{\tilde{I}}) (\underbrace{S^{\dagger N} C^\dagger}_{\tilde{I}} H^\dagger) | 0 \rangle \\
&\sim \langle 0 | (\tilde{I}\tilde{S}^N) (\underbrace{\tilde{C}C^\dagger}_1) (S^{\dagger N} H^\dagger) | 0 \rangle \\
&\sim \langle 0 | (\tilde{I}\tilde{S}^N) T (S^{\dagger N} H^\dagger) | 0 \rangle + \langle 0 | (\tilde{I}\tilde{S}^N) (S^{\dagger N} H^\dagger) | 0 \rangle,
\end{aligned} \tag{20}$$

where the latter term arises from the canonical anticommutator of \tilde{C} and C^\dagger . The result is recognized as consisting of a matrix element and an overlap, respectively, of seniority

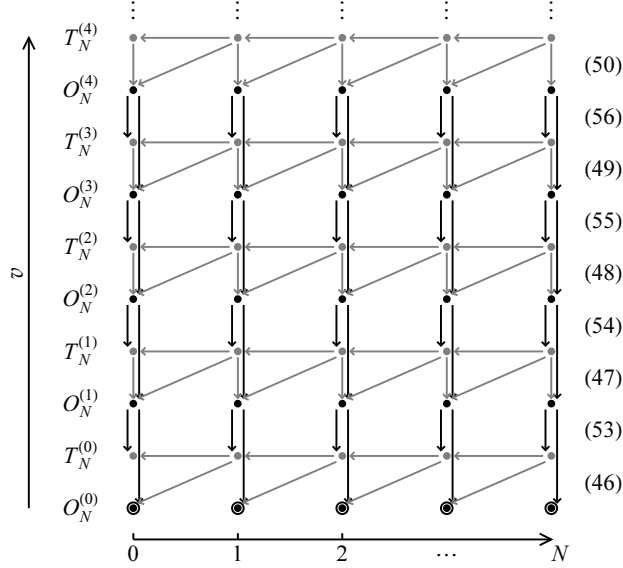


Figure 1: Schematic recurrence network for the calculation of one-body operator reduced matrix elements $T_N^{(v)}$ and overlaps $O_N^{(v)}$ in the generalized seniority scheme, as described by (19) and (21). Equation numbers are indicated at right for the explicit recurrence relations (Secs. 5 and 6) appropriate to each generalized seniority. The seed values $O_N^{(0)}$ (circled) are given by (22). Each point (except for the seed values) represents multiple quantities $T_N^{(v)}[\dots]$ or $O_N^{(v)}[\dots]$, distinguished by the single-particle level and angular-momentum coupling labels.

$v - 1$. The recurrence relation thus has the form

$$O_N^{(v)} \sim T_N^{(v-1)} + O_N^{(v-1)}. \quad (21)$$

The recurrence relations of the form (19) and (21), to be set out in detail in Secs. 5 and 6, allow any matrix element $T_N^{(v)}$ or overlap $O_N^{(v)}$ to ultimately be reexpressed in terms of the norms of states $|S^k\rangle$ of generalized seniority zero, *i.e.*, the $O_k^{(0)}$ ($k = 0, 1, \dots, N$). These constitute the seed values for the recurrence. The recurrence network for evaluating a given $T_N^{(v)}$ or $O_N^{(v)}$ is shown schematically in Fig. 1. The actual recurrence relations involve sums over single-particle indices and over angular momenta for intermediate couplings.

The overlaps $O_N^{(0)}$ are given [3, 13], in terms of the coefficients α_c defining the S pair in (2), by

$$O_N^{(0)} = (N!)^2 \sum_{M \in \mathcal{P}(N,D)} \left[\prod_c \alpha_c^{2M_c} \binom{\Omega_c}{M_c} \right]. \quad (22)$$

The sum is over all ordered partitions $M = (M_1, M_2, \dots, M_D)$ of the integer N into D terms M_c ($\sum_c M_c = N$), where D is the number of active single-particle levels. That is, the sum is over all possible ways in which N pairs may be distributed over the D levels.

Only Pauli-allowed occupancies, $M_c \leq \Omega_c$, contribute, where $\Omega_c = (2c + 1)/2$ is the pair degeneracy of the level.

4. Commutator algebra

In order to carry out the commutation scheme for the elementary one-body operator matrix elements $T_N^{(v)}$, as outlined in Sec. 3, it is necessary to reorder various factors within spherical tensor coupled products. For each value of the generalized seniority v being considered, it is seen from (17)–(18) that commutators of the form $[\tilde{A}, F^{f\dagger}]$ and $[T, F^{f\dagger}]$ will be needed, where $F^{f\dagger}$ is the fermionic cluster creation operator containing v creation operators. That is, $F^\dagger = (A^\dagger \times \dots) \times A^\dagger$ or $((A^\dagger \times \dots) \times A^\dagger) \times C^\dagger$. A straightforward approach is provided by the coupled commutator methods of Chen *et al.* [28], as summarized in this section. All such commutators for $v \leq 4$ (some of which may be found in Refs. [3, 4, 22, 27, 28]) are collected in coupled form below.

The spherical tensor *coupled commutator* [27] is defined by

$$[A^a, B^b]_\varepsilon^e = \sum_{\alpha\beta} (a\alpha b\beta | e\varepsilon) [A_\alpha^a, B_\beta^b]. \quad (23)$$

Since fermionic creation operators obey a canonical *anticommutation* relation, it is more useful in the present context to introduce the *graded coupled commutator*, developed by Chen *et al.* [28], in which the commutation bracket is defined by

$$[A_\alpha^a, B_\beta^b] = A_\alpha^a B_\beta^b - \theta_{ab} B_\beta^b A_\alpha^a, \quad (24)$$

that is, the *commutator* ($\theta_{ab} = +1$) if either angular momentum a or b is integer (quasi-bosonic) but the *anticommutator* ($\theta_{ab} = -1$) if both angular momenta a and b are odd half-integer (quasi-fermionic). [Note $\theta_{ab} \neq \theta(ab)$.] The quantity $[A^a, B^b]^e$ itself constitutes a spherical tensor, indeed, manifestly so, since it may be expressed in terms of coupled products of A^a and B^b as

$$[A^a, B^b]^e = (A^a \times B^b)^e - \theta_{ab} (-)^{e-a-b} (B^b \times A^a)^e. \quad (25)$$

This provides the basic relation for reordering factors within coupled products. The use of coupled commutators thus circumvents the cumbersome process of uncoupling products of operators, commuting the components, and recoupling the result. The commutator has the symmetry (or antisymmetry) property

$$[B^b, A^a]^e = -\theta_{ab} (-)^{e-a-b} [A^a, B^b]^e \quad (26)$$

under interchange of its arguments.

The canonical anticommutation property for fermionic creation and annihilation operators, $[C_{a,\alpha}, C_{b,\beta}^\dagger] = \delta_{ab}\delta_{\alpha\beta}$ (recall this is the graded commutator), is written in coupled form as

$$[\tilde{C}_a, C_b^\dagger]^e = \hat{a}\delta_{ab}\delta_{e0}. \quad (27)$$

Any coupled commutator of more complicated operators can be reduced to (27) by repeated application of the coupled commutator product rule

$$[A^a, (C^c \times D^d)^f]^g = \sum_h \begin{bmatrix} c & d & f \\ g & a & h \end{bmatrix} ([A^a, C^c]^h \times D^d)^g + \sum_h (-)^{d+g-f-h} \theta_{ac} \begin{bmatrix} c & d & f \\ a & g & h \end{bmatrix} (C^c \times [A^a, D^d]^h)^g, \quad (28)$$

which applies for arbitrary spherical tensor operators A^a , C^c , and D^d . The quantity in brackets is the unitary 6- j symbol,

$$\begin{bmatrix} a & b & c \\ d & e & f \end{bmatrix} = (-)^{a+b+d+e} \hat{c} \hat{f} \left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\}, \quad (29)$$

commonly denoted by $U(abed; cf)$.

Commutators of the one-body operator T with the creation operators for fermion clusters are obtained by repeated application of the product rule (28):

$$[T_{ab}^e, C_c^\dagger]^d = \theta(cde) \frac{\hat{e}}{\hat{d}} \delta_{bc} \delta_{ad} C_d^\dagger \quad (30)$$

$$[T_{ab}^e, A_{cd}^{f\dagger}]^g = \bar{\mathbb{P}}(cd; f) \theta(cdeg) \frac{\hat{e} \hat{f}}{\hat{d} \hat{g}} \delta_{bd} \begin{bmatrix} f & e & g \\ a & c & d \end{bmatrix} A_{ac}^{g\dagger} \quad (31)$$

$$[T_{rs}^t, (A_{ab}^{e\dagger} \times C_c^\dagger)^g]^h = \sum_x \bar{\mathbb{P}}(ab; e) \theta(abtx) \frac{\hat{e} \hat{t}}{\hat{b} \hat{x}} \delta_{bs} \quad (32)$$

$$\begin{aligned} & \times \begin{bmatrix} e & c & g \\ h & t & x \end{bmatrix} \begin{bmatrix} e & t & x \\ r & a & b \end{bmatrix} (A_{ra}^{x\dagger} \times C_c^\dagger)^h \\ & + \theta(ght) \frac{\hat{t}}{\hat{r}} \delta_{cs} \begin{bmatrix} e & c & g \\ t & h & r \end{bmatrix} (A_{ab}^{e\dagger} \times C_r^\dagger)^h \\ [T_{rs}^t, (A_{ab}^{e\dagger} \times A_{cd}^{f\dagger})^g]^h &= \sum_x [1 + \theta(efg) \mathbb{P}(abe \leftrightarrow cdf)] \bar{\mathbb{P}}(cd; f) \\ & \times \theta(cdfght) \frac{\hat{f} \hat{t}}{\hat{d} \hat{x}} \delta_{ds} \begin{bmatrix} e & f & g \\ t & h & x \end{bmatrix} \begin{bmatrix} f & t & x \\ r & c & d \end{bmatrix} (A_{ab}^{e\dagger} \times A_{rc}^{x\dagger})^h. \end{aligned} \quad (33)$$

The exchange symbol $\bar{\mathbb{P}}(ab; e)$ (e.g., Refs. [3, 27]) indicates that the following expression should be expanded to consist of *two* terms related by interchange of the indices a and b , as

$$\bar{\mathbb{P}}(ab; e) f(a, b) = f(a, b) - \theta(abe) f(b, a), \quad (34)$$

and $\mathbb{P}(abc \leftrightarrow xyz)$ indicates interchange of the indices abc with xyz .

Commutators of the pair annihilation operator \tilde{A} with the creation operators for

fermion clusters are likewise obtained by application of the product rule (28):

$$[\tilde{A}_{ab}^e, C_c^\dagger]^d = \frac{\hat{e}}{d} \delta(ab; cd; e) \tilde{C}_d \quad (35)$$

$$[\tilde{A}_{ab}^e, A_{cd}^{f\dagger}]^g = \hat{e} \delta_{ef} \delta_{g0} \delta(ab; cd; e) \quad (36)$$

$$\begin{aligned} & - \bar{\mathbb{P}}(cd; f) \bar{\mathbb{P}}(ab; e) \theta(adef) \frac{\hat{e}\hat{f}}{\hat{b}\hat{g}} \delta_{bc} \begin{bmatrix} e & f & g \\ d & a & b \end{bmatrix} T_{da}^g \\ [\tilde{A}_{rs}^t, (A_{ab}^{e\dagger} \times C_c^\dagger)^g]^h = & - \theta(ght) \frac{\hat{g}}{h} \delta_{et} \delta_{ch} \delta(ab; rs; e) C_h^\dagger \end{aligned} \quad (37)$$

$$\begin{aligned} & + \bar{\mathbb{P}}(rs; t) \bar{\mathbb{P}}(ab; e) \theta(egrt) \frac{\hat{e}\hat{t}}{\hat{a}\hat{b}} \delta_{ah} \delta_{br} \delta_{cs} \begin{bmatrix} c & e & g \\ a & t & b \end{bmatrix} C_h^\dagger + \tilde{\mathcal{N}} \\ [\tilde{A}_{rs}^t, (A_{ab}^{e\dagger} \times A_{cd}^{f\dagger})^g]^h = & [1 + \theta(efg) \mathbb{P}(abe \leftrightarrow cdf)] \frac{\hat{g}}{h} \delta_{eh} \delta_{ft} \delta(cd; rs; f) A_{ab}^{h\dagger} \\ & - \bar{\mathbb{P}}(rs; t) \bar{\mathbb{P}}(cd; f) \bar{\mathbb{P}}(ab; e) \hat{e}\hat{f}\hat{g}\hat{t} \delta_{br} \delta_{ds} \begin{Bmatrix} t & h & g \\ d & c & f \\ b & a & e \end{Bmatrix} A_{ac}^{h\dagger} + \tilde{\mathcal{N}}, \end{aligned} \quad (38)$$

where we adopt the shorthand notation

$$\delta(ab; cd; e) = \delta_{ac} \delta_{bd} - \theta(abe) \delta_{ad} \delta_{bc}. \quad (39)$$

The 9- j symbol arises as a sum over products of 6- j symbols from (28), by identity (9.8.5) of Ref. [30]. In (37) and (38), $\tilde{\mathcal{N}}$ represents additional normal-ordered terms containing at least one annihilation operator, which are not explicitly needed for the present calculations, since in Sec. 5 these commutators act directly on the vacuum.

Commutators involving the time-reversed adjoint of the creation operator for a fermionic cluster also arise in (18), from \tilde{G}^g . However, these may be converted into commutators of the type considered above by use of the relation

$$(\widetilde{A^a \times B^b})^{e\dagger} = (-)^{e-a-b} (\tilde{B}^{b\dagger} \times \tilde{A}^{a\dagger})^e, \quad (40)$$

and therefore

$$[\widetilde{A^a, B^b}]^{e\dagger} = (-)^{e-a-b} [\tilde{B}^{b\dagger}, \tilde{A}^{a\dagger}]^e. \quad (41)$$

5. Recurrence relations for matrix elements of one-body operators

The recurrence relations for $T_N^{(v)}$ are obtained by applying the commutation scheme outlined in Sec. 3 to the one-body operator reduced matrix element defined by (15). The requisite commutators are [22]

$$[S^{\dagger N}, T_{cd}^f]^f = N \alpha_d A_{cd}^{f\dagger} S^{\dagger N-1} \quad (42)$$

$$[S^{\dagger N}, \tilde{A}_{cd}^f]^f = -\alpha_c \hat{c} \delta_{cd} \delta_{f0} N S^{\dagger N-1} - \alpha_c N S^{\dagger N-1} T_{cd}^f + \theta(cdf) \alpha_d N T_{dc}^f S^{\dagger N-1}, \quad (43)$$

which follow from (31) and (36), respectively, by induction on N . The general recurrence relation

$$\begin{aligned}
\underbrace{\langle S^N G^g \| T_{rs}^t \| S^N F^f \rangle}_{T_N^{(v)}[\dots]} &= (-)^{f-t-g} \hat{g} \underbrace{\langle S^N G^g | S^N H^g \rangle}_{O_N^{(v)}[\dots]} - N^2 \alpha_s^2 \underbrace{\langle S^{N-1} G^g \| T_{rs}^t \| S^{N-1} F^f \rangle}_{T_{N-1}^{(v)}[\dots]} \\
&- \sum_x \frac{1}{2} N \alpha_s \alpha_x \hat{f} \hat{x} \underbrace{\langle S^{N-1} (A_{xx}^0 I^f) | S^{N-1} F^f \rangle}_{O_{N-1}^{(v)}[\dots]} - N^2 \alpha_r \alpha_s \hat{f} \underbrace{\langle S^{N-1} E^f | S^{N-1} F^f \rangle}_{O_{N-1}^{(v)}[\dots]} \\
&- N^2 \alpha_r^2 \hat{f} \hat{r} \delta_{rs} \delta_{fg} \delta_{t0} \underbrace{\langle S^{N-1} G^g | S^{N-1} F^f \rangle}_{O_{N-1}^{(v)}[\dots]} \quad (44)
\end{aligned}$$

is obtained, in terms of new fermion clusters defined by the coupled commutators

$$\begin{aligned}
E^{f\dagger} &= [T_{rs}^t, G^{g\dagger}]^f \\
H^{g\dagger} &= [T_{rs}^t, F^{f\dagger}]^g \\
I^{f\dagger} &= [\tilde{A}_{rs}^t, G^{g\dagger}]^f.
\end{aligned} \quad (45)$$

Note that each state appearing in the matrix element and overlaps on the right hand side of (44) is, like the original states $|S^N F^f\rangle$ and $|S^N G^g\rangle$, also of generalized seniority v . In particular, the cluster creation operators $E^{f\dagger}$ and $H^{g\dagger}$ each again contain v fermion creation operators, and, although $I^{f\dagger}$ contains $v-2$ fermion creation operators, it appears multiplied by a pair creation operator $A_{xx}^{0\dagger}$, and the combination $A_{xx}^{0\dagger} I^{f\dagger}$ again carries generalized seniority v . The *matrix element* $T_N^{(v)}$ has thus been recast in terms of an *overlap* $O_N^{(v)}$ of the same N and v , as well as a matrix element $T_{N-1}^{(v)}$ and overlaps $O_{N-1}^{(v)}$ of lower pair number, providing the basis for recursive calculation with respect to pair number.

For $v = 0$: As a simple special case, the general recurrence formula (44) gives

$$T_N^{(0)}[(aa)^0] = -N^2 \alpha_a^2 T_{N-1}^{(0)}[(aa)^0] - N^2 \alpha_a^2 \hat{a} O_{N-1}^{(0)}. \quad (46)$$

This may readily be expressed in closed form, in terms of the seed values $O_N^{(0)}$ given in (22), as $T_N^{(0)}[(aa)^0] = \sum_{k=0}^{N-1} (-)^{N+k} (N!^2/k!^2) \alpha_a^{2(N-k)} \hat{a} O_k^{(0)}$.

For $v = 1$: The recurrence relation obtained from (44), with the identifications $F^{f\dagger} \rightarrow C_c^\dagger$ and $G^{g\dagger} \rightarrow C_d^\dagger$, is

$$\begin{aligned}
T_N^{(1)}[d|(rs)^t|c] &= -\hat{t} \delta_{cs} \delta_{dr} O_N^{(1)}[d|d] - N^2 \alpha_s^2 T_{N-1}^{(1)}[d|(rs)^t|c] \\
&- N^2 \theta(rst) \alpha_r \alpha_s \hat{t} \delta_{ds} \delta_{cr} O_{N-1}^{(1)}[c|c] - N^2 \alpha_r^2 \hat{r} \hat{c} \delta_{rs} \delta_{cd} \delta_{t0} O_{N-1}^{(1)}[c|c]. \quad (47)
\end{aligned}$$

The coupled commutators needed for evaluation of $I^{f\dagger}$, $E^{f\dagger}$, and $H^{g\dagger}$ are given by (30) and (35).

For $v = 2$: The recurrence relation, obtained with $F^{f\dagger} \rightarrow A_{ab}^{e\dagger}$ and $G^{g\dagger} \rightarrow A_{cd}^{f\dagger}$, is

$$\begin{aligned}
& T_N^{(2)}[(cd)^f|(rs)^t|(ab)^e] \\
&= \mathbb{P}(ab; e)\theta(ab e)\frac{\hat{e}\hat{t}}{\hat{b}}\delta_{bs}\begin{bmatrix} e & t & f \\ r & a & b \end{bmatrix}O_N^{(2)}[(cd)^f|(ra)^f] - N^2\alpha_s^2T_{N-1}^{(2)}[(cd)^f|(rs)^t|(ab)^e] \\
&\quad - \sum_x \frac{1}{2}N\alpha_s\alpha_x\hat{x}\hat{t}\delta_{ab}\delta_{tf}\delta_{e0}\delta(rs; cd; t)O_{N-1}^{(2)}[(xx)^0|(aa)^0] \\
&\quad - N^2\alpha_r\alpha_s\mathbb{P}(cd; f)\theta(cd et)\frac{\hat{f}\hat{t}}{\hat{d}}\delta_{ds}\begin{bmatrix} f & t & e \\ r & c & d \end{bmatrix}O_{N-1}^{(2)}[(rc)^e|(ab)^e] \\
&\quad - N^2\alpha_r^2\hat{r}\hat{e}\delta_{rs}\delta_{ef}\delta_{t0}O_{N-1}^{(2)}[(cd)^e|(ab)^e]. \quad (48)
\end{aligned}$$

The necessary coupled commutators are given in (31) and (36).

For $v = 3$: The recurrence relation, obtained with $F^{f\dagger} \rightarrow (A_{ab}^{e\dagger} \times C_i^\dagger)^g$ and $G^{g\dagger} \rightarrow (A_{cd}^{f\dagger} \times C_j^\dagger)^h$, is

$$\begin{aligned}
& T_N^{(3)}[(cd)^f j^h|(rs)^t|(ab)^e i^g] \\
&= - \sum_x \mathbb{P}(ab; e)\theta(abghx)\frac{\hat{e}\hat{t}\hat{h}}{\hat{b}\hat{x}}\delta_{bs}\begin{bmatrix} e & i & g \\ h & t & x \end{bmatrix}\begin{bmatrix} e & t & x \\ r & a & b \end{bmatrix}O_N^{(3)}[(cd)^f j^h|(ra)^x i^h] \\
&\quad - \frac{\hat{t}\hat{h}}{\hat{r}}\delta_{is}\begin{bmatrix} e & i & g \\ t & h & r \end{bmatrix}O_N^{(3)}[(cd)^f j^h|(ab)^e r^h] - N^2\alpha_s^2T_{N-1}^{(3)}[(cd)^f j^h|(rs)^t|(ab)^e i^g] \\
&\quad + \sum_x \frac{1}{2}N\alpha_s\alpha_x\theta(gh t)\hat{h}\hat{x}\delta_{ft}\delta_{gj}\delta(cd; rs; f)O_{N-1}^{(3)}[(xx)^0 j^g|(ab)^e i^g] \\
&\quad - \sum_x \frac{1}{2}N\alpha_s\alpha_x\mathbb{P}(rs; t)\mathbb{P}(cd; f)\theta(fhrt)\frac{\hat{f}\hat{t}\hat{x}}{\hat{d}}\delta_{cg}\delta_{dr}\delta_{js}\begin{bmatrix} j & f & h \\ c & t & d \end{bmatrix}O_{N-1}^{(3)}[(xx)^0 c^g|(ab)^e i^g] \\
&\quad - \sum_x N^2\alpha_r\alpha_s\mathbb{P}(cd; f)\theta(cdxt)\frac{\hat{f}\hat{g}\hat{t}}{\hat{d}\hat{x}}\delta_{ds}\begin{bmatrix} f & j & h \\ g & t & x \end{bmatrix}\begin{bmatrix} f & t & x \\ r & c & d \end{bmatrix}O_{N-1}^{(3)}[(rc)^x j^g|(ab)^e i^g] \\
&\quad - N^2\alpha_r\alpha_s\theta(gh t)\frac{\hat{g}\hat{t}}{\hat{r}}\delta_{js}\begin{bmatrix} f & j & h \\ t & g & r \end{bmatrix}O_{N-1}^{(3)}[(cd)^f r^g|(ab)^e i^g] \\
&\quad - N^2\alpha_r^2\hat{r}\hat{g}\delta_{rs}\delta_{gh}\delta_{t0}O_{N-1}^{(3)}[(cd)^f j^g|(ab)^e i^g]. \quad (49)
\end{aligned}$$

The necessary coupled commutators are given in (32) and (37).

For $v = 4$: The recurrence relation, obtained with $F^{f\dagger} \rightarrow (A_{ab}^{e\dagger} \times A_{ij}^{m\dagger})^g$ and $G^{g\dagger} \rightarrow$

$(A_{cd}^{f\dagger} \times A_{kl}^{n\dagger})^h$, is

$$\begin{aligned}
& T_N^{(4)}[(cd)^f(kl)^{n\ h}|(rs)^t|(ab)^e(ij)^{m\ g}] \\
&= \sum_x [1 + \theta(emg)\mathbb{P}(abe \leftrightarrow ijm)]\bar{\mathbb{P}}(ij; m)\theta(ijm)\frac{\hat{m}\hat{t}\hat{h}}{\hat{j}\hat{x}}\delta_{js}\begin{bmatrix} e & m & g \\ t & h & x \end{bmatrix}\begin{bmatrix} m & t & x \\ r & i & j \end{bmatrix} \\
&\quad \times O_N^{(4)}[(cd)^f(kl)^{n\ h}|(ab)^e(ri)^{x\ h}] \\
&\quad - N^2\alpha_s^2 T_{N-1}^{(4)}[(cd)^f(kl)^{n\ h}|(rs)^t|(ab)^e(ij)^{m\ g}] \\
&\quad - \sum_x \frac{1}{2}N\alpha_s\alpha_x[1 + \theta(fnh)\mathbb{P}(cdf \leftrightarrow kln)]\hat{h}\hat{x}\delta_{fg}\delta_{nt}\delta(kl; rs; n) \\
&\quad \times O_{N-1}^{(4)}[(xx)^0(cd)^{g\ g}|(ab)^e(ij)^{m\ g}] \\
&\quad + \sum_x \frac{1}{2}N\alpha_s\alpha_x\bar{\mathbb{P}}(rs; t)\bar{\mathbb{P}}(kl; n)\bar{\mathbb{P}}(cd; f)\hat{f}\hat{n}\hat{g}\hat{h}\hat{t}\hat{x}\delta_{dr}\delta_{ls}\begin{Bmatrix} t & g & h \\ l & k & n \\ d & c & f \end{Bmatrix} \\
&\quad \times O_{N-1}^{(4)}[(xx)^0(ck)^{g\ g}|(ab)^e(ij)^{m\ g}] \\
&\quad - \sum_x N^2\alpha_r\alpha_s[1 + \theta(fnh)\mathbb{P}(cdf \leftrightarrow kln)]\bar{\mathbb{P}}(kl; n)\theta(klngh)\frac{\hat{n}\hat{t}\hat{g}}{\hat{l}\hat{x}}\delta_{ls}\begin{bmatrix} f & n & h \\ t & g & x \end{bmatrix}\begin{bmatrix} n & t & x \\ r & k & l \end{bmatrix} \\
&\quad \times O_{N-1}^{(4)}[(cd)^f(rk)^{x\ g}|(ab)^e(ij)^{m\ g}] \\
&\quad - N^2\alpha_r^2\hat{r}\hat{g}\delta_{rs}\delta_{gh}\delta_{t0}O_{N-1}^{(4)}[(cd)^f(kl)^{n\ g}|(ab)^e(ij)^{m\ g}]. \quad (50)
\end{aligned}$$

The necessary coupled commutators are given in (33) and (38).

6. Recurrence relations for overlaps

The recurrence relations for $O_N^{(v)}$ are obtained by rearranging the factors within (16), as outlined in the commutation scheme of Sec. 3. It is first necessary to recouple the creation operators within $F^{f\dagger}$ and $G^{f\dagger}$, so as to extract a single-fermion creation operator from each cluster, giving

$$\begin{aligned}
F^{f\dagger} &= (C_r^\dagger \times H^{h\dagger})^f \\
G^{f\dagger} &= (C_s^\dagger \times I^{i\dagger})^f.
\end{aligned} \quad (51)$$

These equations define subclusters $H^{h\dagger}$ and $I^{i\dagger}$, each containing $v-1$ fermion creation operators. Then we deduce the general recurrence relation

$$\begin{aligned}
\underbrace{\langle S^N G^f | S^N F^f \rangle}_{O_N^{(v)}[\dots]} &= \sum_x (-)^{f-r-h}\hat{f}^{-1} \begin{bmatrix} s & r & x \\ h & i & f \end{bmatrix} \underbrace{\langle S^N I^i | T_{rs}^x | S^N H^h \rangle}_{T_N^{(v-1)}[\dots]} \\
&\quad + \delta_{rs}\delta_{hi} \underbrace{\langle S^N I^i | S^N H^h \rangle}_{O_N^{(v-1)}[\dots]}. \quad (52)
\end{aligned}$$

The derivation involves only angular momentum recoupling and the canonical anticommutator (27). Each state appearing in the matrix element and overlap on the right hand

side of (52) has generalized seniority $v - 1$. The overlap $O_N^{(v)}$ has therefore been recast in terms of a matrix element $T_N^{(v-1)}$ and overlap $O_N^{(v-1)}$, both of *lower* seniority, providing the basis for recursive calculation with respect to seniority.

For $v = 1$: For this simple special case, with the identifications $F^{f\dagger} \rightarrow C_c^\dagger$ and $G^{f\dagger} \rightarrow C_c^\dagger$, the general recurrence formula (52) reduces to

$$O_N^{(1)}[c|c] = \hat{c}^{-1} T_N^{(0)}[(cc)^0] + O_N^{(0)}. \quad (53)$$

Since $F^{f\dagger}$ and $G^{f\dagger}$ already consist of single-fermion creation operators, the “subcluster creation operators” $H^{h\dagger}$ and $I^{i\dagger}$ are simply the identity operator. From the closed form expression for $T_N^{(0)}$, this gives $O_N^{(1)}[c|c] = \sum_{k=0}^{N-1} (-)^{N+k} (N!^2/k!^2) \alpha_c^{2(N-k)} O_k^{(0)} + O_N^{(0)}$.

For $v = 2$: The recurrence relation, obtained with $F^{f\dagger} \rightarrow A_{ab}^{e\dagger}$ and $G^{f\dagger} \rightarrow A_{cd}^{e\dagger}$, is

$$O_N^{(2)}[(cd)^e|(ab)^e] = \sum_x \theta(abe) \hat{e}^{-1} \begin{bmatrix} c & a & x \\ b & d & e \end{bmatrix} T_N^{(1)}[d|(ac)^x|b] + \delta_{ac} \delta_{bd} O_N^{(1)}[b|b]. \quad (54)$$

The subclusters in (51) are $H^{h\dagger} \rightarrow C_b^\dagger$ and $I^{i\dagger} \rightarrow C_d^\dagger$. Only the $v = 2$ overlaps $O_N^{(2)}[(aa)^e|(aa)^e]$ (e even), $O_N^{(2)}[(cc)^0|(aa)^0]$, and $O_N^{(2)}[(ac)^e|(ac)^e]$ or $O_N^{(2)}[(ca)^e|(ac)^e]$ ($e \neq 0$) are nonvanishing, as may be shown by considering the balance of creation and annihilation operators in the vacuum expectation value for the overlap. Closed form expressions have previously been obtained [22, 23].

For $v = 3$: The recurrence relation, obtained with $F^{f\dagger} \rightarrow (A_{ab}^{e\dagger} \times C_i^\dagger)^g$ and $G^{f\dagger} \rightarrow (A_{cd}^{f\dagger} \times C_j^\dagger)^g$, is

$$O_N^{(3)}[(cd)^f j^g|(ab)^e i^g] = - \sum_x \theta(fgj) \hat{g}^{-1} \begin{bmatrix} j & i & x \\ e & f & g \end{bmatrix} T_N^{(2)}[(cd)^f|(ij)^x|(ab)^e] + \delta_{ij} \delta_{ef} O_N^{(2)}[(cd)^e|(ab)^e]. \quad (55)$$

To decompose $F^{f\dagger}$ and $G^{f\dagger}$ according to (51), it is only necessary to reorder the coupled product so that the single-particle creation operator precedes the pair creation operator [*i.e.*, $A^\dagger \times C^\dagger \rightarrow C^\dagger \times A^\dagger$], which then serves as the subcluster. Thus, $H^{h\dagger} \rightarrow (-)^{g-e-i} A_{ab}^{e\dagger}$ and $I^{i\dagger} \rightarrow (-)^{g-f-j} A_{cd}^{f\dagger}$.

For $v = 4$: The recurrence relation, obtained with $F^{f\dagger} \rightarrow (A_{ab}^{e\dagger} \times A_{ij}^{m\dagger})^g$ and $G^{f\dagger} \rightarrow (A_{cd}^{f\dagger} \times A_{kl}^{n\dagger})^g$, is

$$O_N^{(4)}[(cd)^f (kl)^n g|(ab)^e (ij)^m g] = - \sum_{pqx} \hat{g}^{-1} \theta(abdmngq) \begin{bmatrix} c & a & x \\ p & q & g \end{bmatrix} \begin{bmatrix} a & b & e \\ m & g & p \end{bmatrix} \begin{bmatrix} c & d & f \\ n & g & q \end{bmatrix} T_N^{(3)}[(kl)^n d^q|(ac)^x|(ij)^m b^p] \\ - \delta_{ac} \sum_p \theta(bdmn) \begin{bmatrix} a & b & e \\ m & g & p \end{bmatrix} \begin{bmatrix} a & d & f \\ n & g & p \end{bmatrix} O_N^{(3)}[(kl)^n d^p|(ij)^m b^p]. \quad (56)$$

Here the clusters must be recoupled as $A^\dagger \times A^\dagger \rightarrow C^\dagger \times (C^\dagger \times A^\dagger)$. This gives rise to subclusters $H^{h\dagger} \rightarrow \sum_p (-)^{p-b-m} \begin{bmatrix} a & b & e \\ m & g & p \end{bmatrix} (A_{ij}^{m\dagger} \times C_b^\dagger)^p$ and $I^{i\dagger} \rightarrow \sum_q (-)^{q-d-n} \begin{bmatrix} c & d & f \\ n & g & q \end{bmatrix} (A_{kl}^{n\dagger} \times C_d^\dagger)^q$.

For $v = 5$: The recurrence relation, obtained with $F^{f\dagger} \rightarrow [(A_{ab}^{e\dagger} \times A_{ij}^{m\dagger})^g \times C_p^\dagger]^u$ and $G^{f\dagger} \rightarrow [(A_{cd}^{f\dagger} \times A_{kl}^{n\dagger})^h \times C_q^\dagger]^u$, is

$$\begin{aligned} O_N^{(5)}[(cd)^f(kl)^n q^u |(ab)^e(ij)^m g p^u] = \\ - \sum_x \hat{u}^{-1} \theta(uqh) \begin{bmatrix} q & p & x \\ g & h & u \end{bmatrix} T_N^{(4)}[(cd)^f(kl)^m h |(pq)^x |(ab)^e(ij)^m g] \\ + \delta_{pq} \delta_{gh} O_N^{(4)}[(cd)^f(kl)^m g |(ab)^e(ij)^m g]. \end{aligned} \quad (57)$$

In this case, since v is odd, the extraction of a single-fermion creation operator from each cluster requires only the reordering $(A^\dagger \times A^\dagger) \times C^\dagger \rightarrow C^\dagger \times (A^\dagger \times A^\dagger)$, hence $H^{h\dagger} \rightarrow (-)^{u-g-p} (A_{ab}^{e\dagger} \times A_{ij}^{m\dagger})^g$ and $I^{i\dagger} \rightarrow (-)^{u-h-q} (A_{cd}^{f\dagger} \times A_{kl}^{n\dagger})^h$.

7. Matrix elements of two-body operators

Once overlaps and matrix elements of one-body operators have been calculated in the generalized seniority scheme, from the recurrence relations established in Secs. 5 and 6, the matrix elements of two-body operators follow in a straightforward fashion. The approach is based, once again, on expressing the matrix element as a vacuum expectation value, followed by commutation of the operators to a more convenient ordering, in which the various terms can be recognized as overlaps and one-body operator matrix elements.

An arbitrary two-body operator may be decomposed as a linear combination of elementary terms of the form $(A_{ab}^{e\dagger} \times \tilde{A}_{cd}^f)^w$. In particular, if W^w is a spherical tensor operator of angular momentum w , then the angular-momentum coupled second-quantized form is

$$W^w = \frac{1}{4} \sum_{\substack{abcd \\ ef}} (1 + \delta_{ab})^{1/2} (1 + \delta_{cd})^{1/2} \hat{w}^{-1} \langle (ab)^e \| W^w \| (cd)^f \rangle_{\text{NAS}} (A_{ab}^{e\dagger} \times \tilde{A}_{cd}^f)^w, \quad (58)$$

where it should be noted that $(A_{ab}^{e\dagger} \times \tilde{A}_{cd}^f)^w = -[(C_a^\dagger \times C_b^\dagger)^e \times (\tilde{C}_c \times \tilde{C}_d)^f]^w$, and where the reduced matrix element is taken with respect to normalized antisymmetrized states $|(ab)_\varepsilon^e \rangle_{\text{NAS}} = (1 + \delta_{ab})^{-1/2} (C_a^\dagger \times C_b^\dagger)_\varepsilon^e |0\rangle$. We note this explicitly to avoid ambiguity with the unnormalized $N = 0$, $v = 2$ basis state of Sec. 2. The expression for the two-body Hamiltonian arises as a special case, with $w = 0$.

Evaluating the matrix element of an elementary two-body operator $(A_{ab}^{e\dagger} \times \tilde{A}_{cd}^f)^w$ as a vacuum expectation value involves only a single commutation, of the form $[\tilde{A}, A^\dagger] \sim T + 1$ [see (36)]. Schematically,

$$\begin{aligned} \langle S^N G \| A^\dagger \tilde{A} \| S^N F \rangle &\sim \langle 0 | (\tilde{G} \tilde{S}^N) (\underbrace{A^\dagger \tilde{A}}_{T+1}) (S^{\dagger N} F^\dagger) | 0 \rangle \\ &\sim \langle 0 | (\tilde{G} \tilde{S}^N \tilde{A}) (\underbrace{A^\dagger S^{\dagger N}}_{T+1} F^\dagger) | 0 \rangle + \langle 0 | (\tilde{G} \tilde{S}^N) T (S^{\dagger N} F^\dagger) | 0 \rangle + \langle 0 | (\tilde{G} \tilde{S}^N) (S^{\dagger N} F^\dagger) | 0 \rangle. \end{aligned} \quad (59)$$

That is, the pair creation and annihilation operators A^\dagger and \tilde{A} , which together constitute the two-body operator, must be decoupled from each other and reassociated with the fermion cluster operators for the two states. If F and G are clusters of generalized

seniority v , then the first term above is recognized as an overlap involving two new clusters, of higher generalized seniority $v + 2$. Let us represent the reduced matrix elements of the fundamental *two-body* operators between generalized seniority basis states of *equal* generalized seniority by $W_N^{(v)}[\dots]$, e.g.,

$$W_N^{(4)}[(cd)^f(kl)^{nh}|(rs)^t(xy)^{zw}|(ab)^e(ij)^{mg}] \equiv \langle S^N(cd)^f(kl)^{nh} || (A_{rs}^{t\dagger} \times \tilde{A}_{xy}^z)^w || S^N(ab)^e(ij)^{mg} \rangle. \quad (60)$$

Then the resulting expression for the two-body operator matrix element is of the form

$$W_N^{(v)} \sim O_N^{(v+2)} + T_N^{(v)} + O_N^{(v)}. \quad (61)$$

The full relation obtained following this commutation scheme is

$$\begin{aligned} \langle S^N G^g || (A_{rs}^{t\dagger} \times \tilde{A}_{xy}^z)^w || S^N F^f \rangle &= \sum_k (-)^{t+f-k} \hat{k} \begin{bmatrix} z & t & w \\ f & g & k \end{bmatrix} \underbrace{\langle S^N I^k | S^N H^k \rangle}_{O_N^{(v+2)}[\dots]} \\ &+ \bar{\mathbb{P}}(xy; z) \bar{\mathbb{P}}(rs; t) \theta(sxw) \frac{\hat{t}\hat{z}}{\hat{r}\hat{w}} \delta_{ry} \begin{bmatrix} t & z & w \\ x & s & r \end{bmatrix} \underbrace{\langle S^N G^g || T_{sx}^w || S^N F^f \rangle}_{T_N^{(v)}[\dots]} \\ &- \hat{f}\hat{t}\delta_{tz}\delta_{fg}\delta_{w0}\delta(rs; xy; t) \underbrace{\langle S^N G^g | S^N F^f \rangle}_{O_N^{(v)}[\dots]}, \quad (62) \end{aligned}$$

in terms of new clusters defined by

$$\begin{aligned} H^{k\dagger} &= (A_{rs}^{t\dagger} \times F^{f\dagger})^k \\ I^{k\dagger} &= (A_{xy}^{z\dagger} \times G^{g\dagger})^k. \end{aligned} \quad (63)$$

To obtain a useful relation, in terms of known overlaps of seniority $v + 2$, it may be necessary to recouple the factors making up the operators $H^{k\dagger}$ and $I^{k\dagger}$, so that these fermion cluster creation operators are of the form used in defining the generalized seniority states in Sec. 2. For instance, for the two-body operator matrix elements involving states of $v = 3$, $\langle S^N I^k | S^N H^k \rangle$ matches the definition of $O_N^{(5)}$ in (5) only after the recoupling $[A^\dagger \times (A^\dagger \times C^\dagger)] \rightarrow [(A^\dagger \times A^\dagger) \times C^\dagger]$.

For reference, let us explicitly write the relations for two-body operator matrix elements for states with generalized seniority $v \leq 3$. These expressions involve the $T_N^{(v)}$ with $v \leq 4$ and $O_N^{(v)}$ with $v \leq 5$, as considered explicitly in Secs. 5 and 6.

For $v = 0$:

$$\begin{aligned} W_N^{(0)}[(rs)^t(xy)^{t0}] &= \hat{t}O_N^{(2)}[(xy)^t|(rs)^t] - \bar{\mathbb{P}}(xy; t) \bar{\mathbb{P}}(rs; t) \frac{\hat{t}}{\hat{r}} \delta_{rx} \delta_{sy} T_N^{(0)}[(rr)^0] - \hat{t}\delta(rs; xy; t) O_N^{(0)}. \quad (64) \end{aligned}$$

For $v = 1$:

$$\begin{aligned}
W_N^{(1)}[d|(rs)^t(xy)^z w|c] \\
&= -\sum_k \theta(ck) \hat{k} \begin{bmatrix} z & t & w \\ c & d & k \end{bmatrix} O_N^{(3)}[(xy)^z d^k|(rs)^t c^k] \\
&\quad + \bar{\mathbb{P}}(xy; z) \bar{\mathbb{P}}(rs; t) \theta(sxw) \frac{\hat{t}\hat{z}}{\hat{r}\hat{w}} \delta_{ry} \begin{bmatrix} t & z & w \\ x & s & r \end{bmatrix} T_N^{(1)}[d|(sx)^w|c] \\
&\quad - \hat{c}\hat{t}\delta_{tz}\delta_{cd}\delta_{w0}\delta(rs; xy; t) O_N^{(1)}[c|c]. \quad (65)
\end{aligned}$$

For $v = 2$:

$$\begin{aligned}
W_N^{(2)}[(cd)^f|(rs)^t(xy)^z w|(ab)^e] \\
&= \sum_k \theta(ek) \hat{k} \begin{bmatrix} z & t & w \\ e & f & k \end{bmatrix} O_N^{(4)}[(xy)^z (cd)^f k|(rs)^t (ab)^e k] \\
&\quad + \bar{\mathbb{P}}(xy; z) \bar{\mathbb{P}}(rs; t) \theta(sxw) \frac{\hat{t}\hat{z}}{\hat{r}\hat{w}} \delta_{ry} \begin{bmatrix} t & z & w \\ x & s & r \end{bmatrix} T_N^{(2)}[(cd)^f|(sx)^w|(ab)^e] \\
&\quad - \hat{e}\hat{t}\delta_{tz}\delta_{ef}\delta_{w0}\delta(rs; xy; t) O_N^{(2)}[(cd)^e|(ab)^e]. \quad (66)
\end{aligned}$$

For $v = 3$:

$$\begin{aligned}
W_N^{(3)}[(cd)^f j^h|(rs)^t(xy)^z w|(ab)^e i^g] \\
&= -\sum_{pqk} \theta(tgk) \hat{k} \begin{bmatrix} z & f & q \\ j & k & h \end{bmatrix} \begin{bmatrix} t & e & p \\ i & k & g \end{bmatrix} \begin{bmatrix} z & t & w \\ g & h & k \end{bmatrix} O_N^{(5)}[(xy)^z (cd)^f q j^k|(rs)^t (ab)^e p i^k] \\
&\quad + \bar{\mathbb{P}}(xy; z) \bar{\mathbb{P}}(rs; t) \theta(sxw) \frac{\hat{t}\hat{z}}{\hat{r}\hat{w}} \delta_{ry} \begin{bmatrix} t & z & w \\ x & s & r \end{bmatrix} T_N^{(3)}[(cd)^f j^h|(sx)^w|(ab)^e i^g] \\
&\quad - \hat{g}\hat{t}\delta_{tz}\delta_{gh}\delta_{w0}\delta(rs; xy; t) O_N^{(3)}[(cd)^f j^g|(ab)^e i^g]. \quad (67)
\end{aligned}$$

8. Conclusion

The calculational framework presented here provides a straightforward and systematic approach to constructing recurrence relations for matrix elements and overlaps in a generalized seniority scheme. Matrix elements of the one-body and two-body multipole operators have been considered explicitly here, but matrix elements of other operators of interest, such as the pair transfer operator [4, 18], may be derived similarly.

Aside from some elementary angular-momentum recoupling, the derivation only requires calculation of commutators of the form $[T, A^\dagger \times \cdots \times A^\dagger]$ (or $[T, A^\dagger \times \cdots \times A^\dagger \times C^\dagger]$ for odd particle number) and $[\bar{A}, A^\dagger \times \cdots \times A^\dagger]$ (or $[\bar{A}, A^\dagger \times \cdots \times A^\dagger \times C^\dagger]$ for odd particle number). This may be accomplished systematically via the coupled commutator product rule (28). Although the process becomes increasingly laborious for larger v (*i.e.*, $v = 5, 6$, and 7 , or higher if needed), it is also well-suited to automation [29].

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